Aquarius CAP Algorithm and Data User Guide

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Contributors

The Aquarius geophysical model functions for the CAP algorithm were developed by Dr. Wenqing Tang; the operational setup and processing of the CAP algorithm was completed by Dr. Alex Fore; the setup of data portal and data transfer was performed by Mrs. Akiko Hayashi.

Date		Version	Changes/Comments
February 20, 2013	Page 8	2.0	Updated the cost function by adding two additional terms to constrain the wind speed and direction retrieval
February 20, 2013	Page 11	2.0	Add 10 to the flag to indicate possible rain contamination
February 20, 2013	Pages 5 and 6	2.0	Include the significant wave height as a modeling parameter for radar backscatter and excess emissivity
June 20, 2014	All	3.0	Include the rain corrections to GMFs of radar backscatter and excess emissivity and provide references to the articles on product validation results.
Sept. 20, 2015	Page 6, 8-11, 13- 27	4.0	Include the rain corrections to GMFs of excess emissivity with rain-induced near surface stratification accounted for by the Rain Impact Model; and provide results of validation in comparison with APDRC Argo-gridded product and in situ data from moored buoys.

Sept. 26, 2018	5.0	The Geophysical Model Functions
		(GMFs) are updated to 4 th order
		harmonics and include the effect of sea
		surface temperature (SST) and stability
		at air-sea interface.
		2. The source of the ancillary sea surface
		temperature (SST) has been changed
		from NOAA OI SST to the SST from the
		Canadian Meteorological Center (CMC).

Contents

I.	Purpose	5
II.	Introduction	e
III.	Geophysical Model Function	6
	Overview of CAP algorithm	
V.	CAP L2 Data and Format	9
ļ	A. File name convention	<u>c</u>
E	B. Description of datasets in HDF	<u>c</u>
	1. CAP outputs	<u>c</u>
	2. Carryover from Aquarius L2 files	
VI.	CAP L3 Data and Format	. 11
VII.	References	. 12

I. PURPOSE

This document provides an overview of the Combined Active-Passive (CAP) Algorithm for the sea surface roughness correction to enable the retrieval of sea surface salinity, wind speed and direction from Aquarius data. The results from the CAP algorithm are output to files in HDF5 format. This document describes the datasets in the files and their format.

II. INTRODUCTION

The measurement principle for salinity remote sensing is based on the response of the L-band (1.413 GHz) sea surface brightness temperatures (T_B) to sea surface salinity [1]. The influence of wind speed on L-band T_B has been shown to be about 0.2 to 0.3 K for one m·s⁻¹ change in wind speed by many field studies [2-7]. To achieve the required 0.2 practical salinity unit (psu) accuracy for Aquarius mission, the impact of sea surface roughness (e.g. wind-generated ripples, foam, and swells) on the observed brightness temperature has to be accurately corrected, ideally to better than one tenth of a degree Kelvin.

The Aquarius radiometer and scatterometer have been fully operating from August 25, 2011 to June 7, 2015. Other than the interruptions caused by a few spacecraft maneuvers, the data acquisition has been continuous. The Aquarius instrument has three antenna beams, operating at about 29, 38 and 46 degrees [8]. Each antenna beam has one radiometer (1.413 GHz), which can acquire the first three Stokes parameters of microwave radiation. The antenna feeds are shared with the scatterometer (1.26 GHz), which acquire the normalized radar cross sections (σ_0) for coand cross-polarizations, including VV, HH, VH and HV polarizations.

The Aquarius radiometers make partial polarimetric measurements for the first three Stokes parameters, I, Q, and U [9]. I and Q correspond to the sum and difference of the vertically polarized brightness temperature (T_{BV}) and horizontally polarized brightness temperature (T_{BH}). T_{BV} and T_{BH} are measures of the power of the vertically polarized electrical field (E_{V}) and horizontally polarized electric field (E_{H}), while the third and fourth Stokes parameters (U and V) signify the correlation between E_{V} and E_{H} :

$$\begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = \begin{bmatrix} T_{BV} + T_{BH} \\ T_{BV} - T_{BH} \\ U \\ V \end{bmatrix} \propto \begin{bmatrix} \left\langle |E_{v}|^{2} \right\rangle + \left\langle |E_{u}|^{2} \right\rangle \\ \left\langle |E_{v}|^{2} \right\rangle - \left\langle |E_{u}|^{2} \right\rangle \\ 2 \operatorname{Re} \left\langle E_{v} E_{u}^{*} \right\rangle \\ 2 \operatorname{Im} \left\langle E_{v} E_{v}^{*} \right\rangle \end{bmatrix}$$

$$(1)$$

The angular brackets denote the ensemble average of the enclosed quantities. Aquarius does not measure the fourth Stokes V.

III. GEOPHYSICAL MODEL FUNCTION

The matchup data using either SSM/I or NCEP wind for binning have been used to develop the geophysical model functions (GMF) for Aquarius [13], which relate the microwave backscatter or excess surface emissivity to the wind speed (w) and direction (ϕ). In addition, we include the NOAA WaveWatch-III Significant Wave Height (SWH), CMORPH rain rate (R), sea surface temperature (SST) from the Canadian Meteorological Center, and air temperature (T_a) from NCEP to develop the GMF and as ancillary for retrieval.

The radar GMF is expressed as:

$$\sigma_{0,p} = \sigma_p^{wind} + \sigma_p^{rain} + \sigma_p^{SST} + \sigma_p^{dT}$$
 (2)

where p stands for VV (V-transmit/V-receive) and HH (H-transmit/H-receive), respectively. The wind/wave induced roughness is modeled in terms of 4th order cosine series:

$$\sigma_p^{wind} = A_{0,p}^{wind}(w, swh)[1 + \sum_{n=1}^4 A_{n,p}^{wind}(w)\cos(n\phi)]$$
 (3)

The residuals after applying the wind/wave correction (i.e. σ_p^{meas} - σ_p^{wind}) are analyzed to model subsequently the effects of rain (Eq. 4), SST (Eq. 5) and the surface stability parameterized in terms of the temperature difference at the interface of air and seawater (i.e. $dT=T_a$ -SST) in Eq. 6.

$$\sigma_p^{rain} = A_{0,p}^{rain}(w, R) + \sum_{n=1}^4 A_{n,p}^{rain}(w, R) \cos(n\phi)$$
 (4)

$$\sigma_p^{SST} = A_{0,p}^{SST}(w, SST) + \sum_{n=1}^4 A_{n,p}^{SST}(w, SST)\cos(n\phi)$$
 (5)

$$\sigma_p^{dT} = A_{0,p}^{dT}(w, dT) + \sum_{n=1}^4 A_{n,p}^{dT}(w, dT) \cos(n\phi)$$
 (6)

The radiometer model function for excessive emissivity is expressed as:

$$\Delta e_p = e_p^{wind} + e_p^{rain} + e_p^{SST} + e_p^{dT} \tag{7}$$

where p stands for V-pol and H-pol. The largest term is from wind/wave induced roughness,

$$e_p^{wind} = e_{0,p}^{wind}(w, swh) + \sum_{n=1}^4 e_{n,p}^{wind}(w)\cos(n\phi)$$
 (8)

The residuals after applying the wind/wave correction are analyzed to model subsequently the effects of rain (Eq. 9), SST (Eq. 10) and the surface stability (Eq. 11).

$$e_p^{rain} = e_{0,p}^{rain}(w, R) + \sum_{n=1}^4 e_{n,p}^{rain}(w, R) \cos(n\phi)$$
 (9)

$$e_p^{SST} = e_{0,p}^{SST}(w, SST) + \sum_{n=1}^4 e_{n,p}^{SST}(w, SST) \cos(n\phi)$$
 (10)

$$e_p^{dT} = e_{0,p}^{dT}(w, dT) + \sum_{n=1}^4 e_{n,p}^{dT}(w, dT) \cos(n\phi)$$
(11)

The third Stokes parameter for the L-band frequency is modeled by the sine function of the wind direction.

Given the GMF for excess surface emissivity, following are the complete descriptions of the radiometer model function, which relates the brightness temperatures to surface salinity (SSS), SST, wind speed and direction, SWH, R, and dT:

$$TB_{V}(SSS,SST,w,\phi,swh,R,dT) = TB_{V}^{flat}(SSS,SST) + SST \cdot \Delta e_{V}(w,\phi,R,SST,dT) \quad (12)$$

$$TB_H(SSS, SST, w, \phi, swh, R, dT) = TB_H^{flat}(SSS, SST) + SST \cdot \Delta e_H(w, \phi, R, SST, dT)$$
 (13)

$$U(SSS, SST, w, \phi) = U_1(w)\sin\phi + U_2(w)\sin2\phi \tag{14}$$

T_{Bflat} is the brightness temperature for flat water surfaces computed using the water dielectric constant model [10, 11,16, 20] for given Reynolds SST and SSS. The subscript "p" stands for the polarization. The impact of ocean waves on L-band brightness temperatures and backscatter from the ocean surface was analyzed in [23].

IV. OVERVIEW OF CAP ALGORITHM

The CAP algorithm retrieves the salinity and wind simultaneously by finding the best-fit solution to minimize the difference between the Aquarius data and the model functions described in Eqs. (2)-(9). The earlier versions of the CAP algorithm [12,13] use different functional forms for the cost function. After gaining more knowledge about the characteristics of the Aquarius L-band microwave data, particularly the weak response of radar backscatter to wind speed near the crosswind direction, we included the last two additional terms in Eq. (10) to constrain the wind speed and direction solutions primarily for near the crosswind directions. Detailed description of the CAP V3.0 retrieval algorithm is provided in [20]. The major updates to V2.0 include improved correction of reflected galactic radiation, geophysical model functions and cost function. The cost function for the CAP Version 3 and 4 algorithm is

$$F_{cap}(SSS, w, \phi) = \sum_{p=V, H} \frac{(T_{Bp} - T_{Bpm})^2}{\Delta T^2} + \sum_{p=V, H} \frac{(\sigma_{0p} - \sigma_{0pm})^2}{(\gamma_p \sigma_{0p})^2} + \frac{(w - w_{NCEP})^2}{\Delta w^2} + \frac{\sin^2[(\phi - \phi_{NCEP})/2]}{\delta^2}$$
(15)

The weighting factors for the Aquarius data are set according to the expected measurement and modeling uncertainties. We let ΔT be the Noise-Equivalent-Delta-T (NEDT) of radiometer and γ_p be 1.4 times of the radar measurement sensitivity (k_{pc}). The values of NEDT and k_{pc} , a function of signal-to-noise ratio, have been pre-computed and saved in the Aquarius L2 data files. The value of Δw is 1.5 ms⁻¹, a rather weak constraint because the accuracy of CAP wind speeds is estimated to be about 0.7 ms⁻¹ [13]. The value of δ is 0.2, which will constrain the wind direction to be within an RMS deviation of 11 degrees from the NCEP wind direction. Our previous analysis [13] indicates that the directional accuracy of the CAP algorithm is about 10 degrees or better for wind speeds of 15 ms⁻¹ or above. The effect of the last term will not impact the accuracy of the CAP wind direction retrieval for high winds, but will help constrain the wind direction solution for low winds, for which the L-band data have a weak response to wind direction.

For the Aquarius data, we applied the conjugate gradient technique using a modified Levenberg-Marquardt algorithm [14] to find the local minima of F_{cap+} . There are in general four local minima (ambiguous solutions). This is due to the expansion of the model function for wind direction by including up to the second harmonics of the cosine series. For each given wind speed solution, there will in general be four direction solutions, except when the relative wind direction is along upwind, or downwind or crosswind. This can be easily understood by considering the special case when the A_1 coefficients are zero in the model functions. If the first

harmonic coefficient A_1 is zero, these four solutions, corresponding to the inversion of $\cos 2\phi$, are ϕ , $-\phi$, $\phi+180^{\circ}$ and 180° - ϕ . If A_1 and e_{B1} are small, then the third and fourth solutions will shift slightly away from $\pm \phi+180^{\circ}$. Note that because the cosine series are even functions, the solution pair, $\pm \phi$, will produce identical values for model functions, and consequently lead to the same SSS and wind speed solutions. The same is true for the $\pm \phi+180^{\circ}$ solution pair.

A nominal technique developed for the current or past spaceborne wind scatterometer and radiometer missions is the use of numerical weather analysis, such as NCEP or European Center for Medium Range Forecasts (ECMWF), or special wind features to assist the selection of solutions [15]. For salinity and wind speed retrievals, the discrimination of ambiguities is a less challenging issue than ocean wind scatterometers or radiometers because what is needed is to separate the four solutions into two pairs, $\pm \phi$ and $\pm \phi$ +180°, which are separated by about 180 degrees. As previously discussed, each pair will have the same SSS and wind speed values. In our analysis, we use the numerical wind analyses to select the solution by selecting the solution with the closest wind direction to NCEP.

V. CAP L2 DATA AND FORMAT

The Aquarius CAP L2 files contain the CAP algorithm outputs and a few datasets in the Aquarius L2 data files, in HDF format.

A. File name convention

The file names are similar to the Aquarius L2 files. The first part of the file name is the same as that in the Aquarius L2 files. We added the extension '.cap' to it.

For example, Q2012001012500.L2_SCI_V5.0.cap, is the file for the data pass started at 01:25:00 UT on day 1, 2012. "L2_SCI_V5.0" indicates the version of Aquarius L2 files used for the CAP processing.

B. Description of datasets in HDF

The datasets in the HDF5 files are part of the root file, not in a "Aquarius Data" group. Each dataset has 4083 blocks for 3 antenna beams.

A simple way to separate the data from ascending and descending passes for ocean observations is to use the first array index of the dataset. If the first array index is smaller (greater) than 2042, then the data are from ascending (descending) orbits.

1. CAP outputs

The CAP data and critical time and location data sets are outlined below.

Dataset Size Format Unit Valid range Description	Dataset	Size	Format	Unit	Valid range	Description
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	(Block, Beam)				
Sec	Dataset {4083}	double float	Seconds	0.d0 to 86399.999999d0	Block time in seconds of day
beam_clat	Dataset {4083, 3}	float	Degree	-90 to 90	Latitude of footprint
beam_clon	Dataset {4083, 3}	float	Degrees	-180 to 180	Longitude of footprint
SSS_cap	Dataset {4083, 3}	float	Psu	0 to 50	SSS from the CAP algorithm
SSS_cap_rc	Dataset {4083,3}	Float	Psu	0 to 50	SSS from the CAP with rain correction if RR>0; SSS_cap_rc is identical to SSS_cap if no rain (RR=0), or there is no rain data matchup with Aquarius
SSS_cap_v	Dataset {4083, 3}	float	Psu	0 to 50	SSS retrieved from the V-pol TB using the scat_wind_speed for excess surface emissivity correction
wind_speed_cap	Dataset {4083, 3}	float	Meters per sec	Greater than 0	Wind speed retrieved from the CAP algorithm
wind_dir_cap	Dataset {4083, 3}	float	Degrees	-180 to 180	Wind direction retrieved from the CAP algorithm
cap_flag	Dataset {4083, 3}	H5T_NA TIME_U CHAR		0 to 5, 10 to 15 and 100 [*]	Flag for CAP retrieval
scat_wind_speed	Dataset {4083, 3}	float	Meters per sec	Greater than 0	Wind speed retrieved from the Aquarius scatterometer data using the NCEP wind direction as ancillary information

wind_dir_cap is the wind direction retrieved from the Aquarius data, and is the direction from with respect to the north in clockwise direction. Its error is less than 20 degrees RMS at greater than 12 m/s wind speeds for beam 1 and 10 m/s for beams 2 and 3.

cap_flag: The flag for CAP algorithm retrieval with the values of 0, 1, and 2 for valid SSS retrieval and 3 and 4 for invalid SSS retrieval. If the matchup rain rate (RR) from SSMIS or WindSat is greater than zero, we add 10 to the flag to indicate possible rain contamination.

- 0 for abs(wind_speed_cap-anc_wind_speed) <15 m/s
- 1 for abs(wind_speed_cap-anc_wind_speed) <30 m/s

- 2 for abs(wind speed cap-anc wind speed) >30 m/s
- 3 for wind speed cap <0 or sss cap < 0 or sss cap > 50
- 4 for no retrieval
- 5 for TBerr >= 0.4 K, where $TB_{err} = \sqrt{\left(TB_V^{meas.} TB_V^{mod.}\right)^2 + \left(TB_H^{meas.} TB_H^{mod.}\right)^2}$
- 10 for abs(wind_speed_cap-anc_wind_speed) <15 m/s and RR>0
- 11 for abs(wind_speed_cap-anc_wind_speed) <30 m/s and RR>0
- 12 for abs(wind_speed_cap-anc_wind_speed) >30 m/s and RR>0
- 13 for wind_speed_cap <0 or sss_cap < 0 or sss_cap > 50 and RR>0
- 14 for no retrieval and RR >0
- 15 for TBerr >= 0.4 K and RR >0

*We added 100 to the cap_flag if abs(rad_TaV-rad_TfV)>= 1 or abs(rad_TaH-rad_TfH)>= 1.

2. Carryover from Aquarius L2 files

The following are datasets carried over from the Aquarius L2 files. They are included for ease of comparison with the CAP products.

Dataset	Size (Block, Beam)	Unit	Description
SSS	Dataset {4083, 3}	Psu	SSS in the Aquarius L2 files
anc_SSS	Dataset {4083, 3}	Psu	Ancillary (HYCOM) SSS in the Aquarius
			L2 files
anc_surface_temp	Dataset {4083, 3}	Kelvin	SST in the Aquarius L2 files
anc_wind_speed	Dataset {4083, 3}	Meters per sec	Ancillary (NCEP) wind speed in the
			Aquarius L2 files
anc_wind_dir	Dataset {4083, 3}	Degrees	Ancillary wind direction (NCEP) in the
			Aquarius L2 files
scat_land_frac	Dataset {4083, 3}		Scatterometer land fraction in the
			Aquarius L2 files (unitless between 0
			and 1)
scat_ice_frac	Dataset {4083, 3}		Scatteroemter ice fraction in the
			Aquarius L2 files (unitless between 0
			and 1)
land_frac	Dataset {4083, 3}		Radiometer land fraction in the
			Aquarius L2 files (unitless between 0
			and 1)
ice_frac	Dataset {4083, 3}		Radioemter ice fraction in the Aquarius
			L2 files (unitless between 0 and 1)

VI. CAP L3 DATA AND FORMAT

The Aquarius CAP L3 data contain monthly and weekly maps on 1°x1° grid for both SSS_cap and SSS_cap_rc, in netcdf format. L3 data are created using Gaussian weighting with half-power and searching distances at 75 and 111 km, respectively. The filtering criteria for transferring data

from Level 2 to Level 3 are: land_frac < 0.01, ice_frac < 0.0005, anc_surface_temp > 273, and cap_flag < 3 or 10<=cap_flag < 13, in addition to checking the radiometer flag included in Aquarius L2 files for non-nominal navigation (bit-12), and pointing anomaly (bit-16).

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